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(1) A first-principles computer program was completed for calculations of surface properties of semiconductors, and of the interaction of a scanning-tunneling-microscopy tip with a semiconductor surface. We plan to use this program in studies of surface adsorption and diffusion, of the theoretical interpretation of STM, and of atomic manipulation with a STM tip. Since it involves state-of-the-art methods (norm-conserving pseudopotentials, conjugate-gradient techniques, etc.) and consists of 3340 lines of original code, writing it was a nontrivial task.

We calculated the perturbation of the electronic structure of a Si(100) surface by an STM tip in a normal experiment (~2 volts applied at a separation of ~8 Å) and found it to be negligibly small. This rules out a proposed explanation of the symmetric-dimer images seen in defect-free regions of the Si(100) surface. More recently we have extended the calculations to treat geometrical distortions, the effect of stronger fields, and the motion of an atom pulled out of the surface in an atomic manipulation experiment. In collaboration with Michael Weimer, an STM experimentalist, we studied the influence of the internal image potential in STM on semiconductors.

(2) Using a completely independent first-principles program for clusters, that was developed partly by us at Texas A&M (in association with Cray Research, which has since incorporated it into Cray's UniChem package), we generated first-principles-based models for molecular dynamics computer simulations that are more reliable than the models we used in the past. These new models consist of a third-neighbor tight-binding Hamiltonian and a three-body potential, with parameters fitted to the first-principles cluster calculations. We used the model of Si alone to obtain a total-energy surface for Si(100), and to study the dynamic and static structures of Si(100) at low, medium, and high temperature. More recently, a similar model for Si-As and As-As interactions has been used to study the deposition of As on a Si surface.